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FAN 2002:332188

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updated search

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PATENT FAMILY INFORMATION:

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IT **405172-14-7P 405172-81-8P 405172-82-9P**
405172-83-0P 405172-84-1P 405173-01-5P
405173-02-6P 405173-43-5P 405173-45-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

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(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolylmethylaminotetrahydroquinolines and related compds. as chemokine receptor binding agents)

RN 405172-14-7 CAPLUS

CN 1,4-Benzenedimethanamine, N,N'-bis(1H-benzimidazol-2-ylmethyl)-N,N'-bis(5,6,7,8-tetrahydro-8-quinolinyl)-, tetrahydrobromide (9CI) (CA INDEX NAME)

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PATENT FAMILY INFORMATION:

FAN 2002:220575

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NEWS 6	DEC 14	CA/CAplus to be enhanced with updated IPC codes
NEWS 7	DEC 21	IPC search and display fields enhanced in CA/CAplus with the IPC reform
NEWS 8	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS 9	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 10	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS 11	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 12	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS 13	JAN 30	Saved answer limit increased

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:08:48 ON 31 JAN 2006

=> file registry

10799386

1/30/06

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:08:59 ON 31 JAN 2006
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JAN 2006 HIGHEST RN 873057-98-8
DICTIONARY FILE UPDATES: 30 JAN 2006 HIGHEST RN 873057-98-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

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**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information. *
*                                                                    *
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Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


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FULL SEARCH INITIATED 12:10:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    13621 TO ITERATE
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1/30/06

100.0% PROCESSED 13621 ITERATIONS 86 ANSWERS
SEARCH TIME: 00.00.01

L2 86 SEA SSS FUL L1

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 167.38 167.59

FILE 'CAPLUS' ENTERED AT 12:10:26 ON 31 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 31 Jan 2006 VOL 144 ISS 6
FILE LAST UPDATED: 30 Jan 2006 (20060130/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

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L3 3 L2

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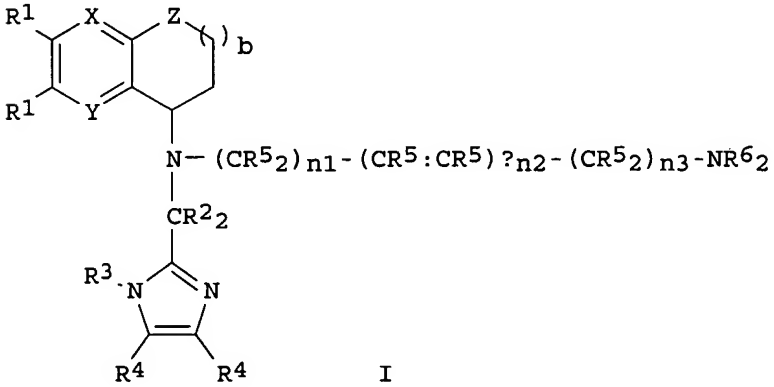
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 μM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. It is also stated that the compds. I behave in a manner similar to 1,1'-[1,4-phenylene-bis(methylene)]-bis-1,4,8,11-tetraazacyclotetradecane (AMD3100) which showed to elevate progenitor cell levels (data given). Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

AN 2004:80349 CAPLUS
DN 140:146136

TI Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary; Kaller, Al; Harwig, Curtis; Skerlj, Renato; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher D.; Di Fluri, Maria R.
PA USA

SO U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of U.S. Ser. No. 446,170.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004019058	A1	20040129	US 2003-457034	20030606
US 2003220341	A1	20031127	US 2002-329329	20021223
WO 2004106493	A2	20041209	WO 2004-US15977	20040521
WO 2004106493	A3	20050825		

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-342716P P 20011221

	US 2002-350822P	P	20020117
	US 2002-329329	A2	20021223
	US 2003-446170	A2	20030523
	US 2003-457034	A	20030606

OS MARPAT 140:146136

IT **558441-51-3P**

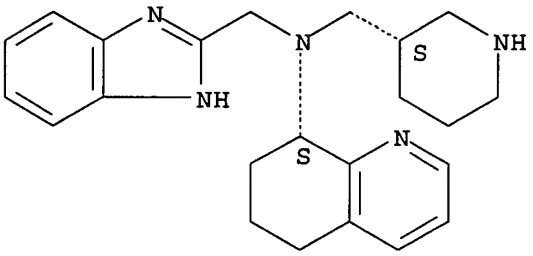
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of chemokine receptor binding benzimidazolylmethyl tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)

RN 558441-51-3 CAPLUS

CN 8-Quinolinamine, N-(1H-benzimidazol-2-ylmethyl)-5,6,7,8-tetrahydro-N-[(3R)-3-piperidinylmethyl]-, trihydrobromide, (8R)-rel- (9CI) (CA INDEX NAME)

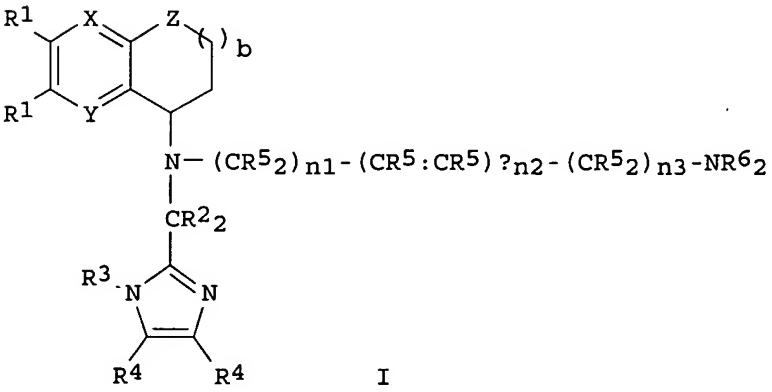
Relative stereochemistry.



●3 HBr

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

GI



I

AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 μM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

AN 2003:532661 CAPLUS
DN 139:101128

TI Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary J.; Skerlj, Renato T.; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria
PA Anormed Inc., Can.; et al.

SO PCT Int. Appl., 360 pp.
CODEN: PIXXD2
DT Patent
LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003055876	A1	20030710	WO 2002-US41407	20021223
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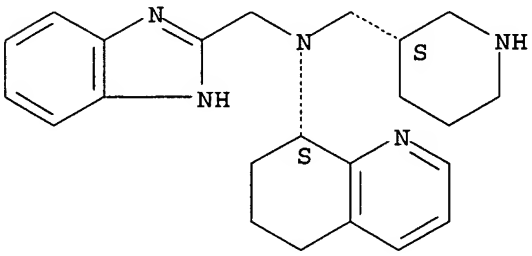
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2467718	AA	20030710	CA 2002-2467718	20021223
	AU 2002357379	A1	20030715	AU 2002-357379	20021223
	BR 2002015050	A	20041013	BR 2002-15050	20021223
	EP 1465889	A1	20041013	EP 2002-805977	20021223
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	JP 2005518397	T2	20050623	JP 2003-556406	20021223
	NO 2004002578	A	20040907	NO 2004-2578	20040618
PRAI	US 2001-342716P	P	20011221		

US 2002-350822P P 20020117
WO 2002-US41407 W 20021223
OS MARPAT 139:101128
IT **558441-51-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of chemokine receptor binding benzimidazolylmethyl tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)
RN 558441-51-3 CAPLUS
CN 8-Quinolinamine, N-(1H-benzimidazol-2-ylmethyl)-5,6,7,8-tetrahydro-N-[(3R)-3-piperidinylmethyl]-, trihydrobromide, (8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●3 HBr

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
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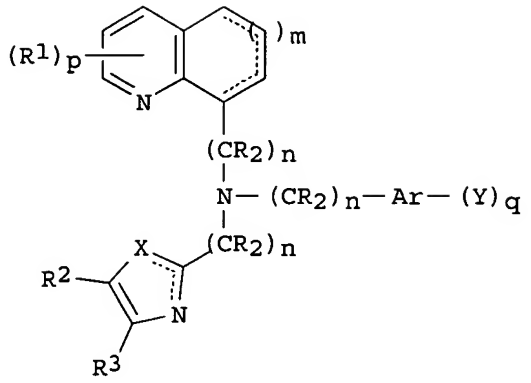

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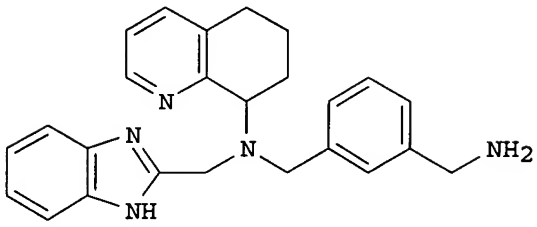

II

AB Title compds. I [wherein ring A optionally comprises a heteroatom selected from N, O, or S; R1-R3 = non-interfering substituents; R4 and R5 = independently H or (un)substituted alkyl, alkenyl, alkynyl, or acyl; or 2 R5 may form a cyclic amine, optionally containing 1 or more N, O, and/or S; R = independently H or alkyl; X = O or S or (un)substituted C or N; Y = independently halo, OH, SH, SO, SO2, non-N containing organic moiety, (CH2)xCN, (CR2)xNR52, (CR2)xNR(CR2)xNRR4, (CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xCO(CR2)xNR52, (CR2)xCO(CR2)xNR(CR2)xNRR4, (CR2)xCO(CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNRR4, (CR2)xNRCO(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNR(CR2)xNR(CR2)xNR(CR2)xNR52, CH:NZ, (CR2)xZ, NR(CR2)xZ, (CR2)xNROH, (CR2)xCONROH, or (CR2)xCR:NOH; or 2 Y groups may be connected to form a fused ring with Ar; Z = (un)substituted (hetero)aryl; Ar = (hetero)aryl; m = 0-2; n = 0-2; p = 0-4; q = 0-3; x = 0-4; with provisos; and pharmaceutically acceptable salts and pro-drugs thereof] were prepared as modulators of chemokine receptor activities. For example, reductive addition of 3-cyanobenzaldehyde to 8-amino-5,6,7,8-tetrahydroquinoline using sodium triacetoxyborohydride in CH2Cl2 afforded N-(5,6,7,8-tetrahydro-8-quinolinyl)-3-cyanobenzylamine (81%). Alkylation with N-(tert-butoxycarbonyl)-2-chloromethylbenzimidazole using N,N-diisopropylethylamine and KI in MeCN (88%), followed by hydrogenation in the presence of Raney nickel (79%), gave the tertiary amine II (AMD9679). Compds. of the invention tested for inhibition of HIV-1 NL4.3 or IIIB replication in MT-4 cells exhibited EC50 values of 0.002 μM/mL to 20.0 μM/mL. Thus, I are useful for the treatment of human immunodeficiency virus (HIV) and/or feline immunodeficiency virus (FIV).

AN 2002:332188 CAPLUS

DN 136:355235

TI Preparation of tertiary N-(5,6,7,8-tetrahydro-8-quinolinyl)-N-(1H-benzimidazol-2-ylmethyl)amines and analogs as chemokine receptor modulators for treatment of HIV or FIV

IN Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David;

Wilson, Trevor R.; Crawford, Jason; Mceachern, Ernest J.; Atsman, Berm; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria
PA Anormed Inc., Can.
SO PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002034745	A1	20020502	WO 2001-US29590	20010919
WO 2002034745	C1	20030918		
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CA 2421796	AA	20020502	CA 2001-2421796	20010917
EP 1317451	A1	20030611	EP 2001-975290	20010917
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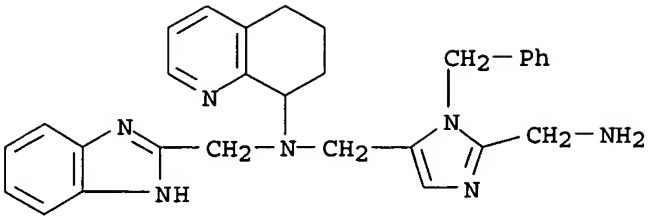
BR 2001013932	A	20030624	BR 2001-13932	20010917
NZ 524651	A	20050826	NZ 2001-524651	20010917
AU 2001094628	A5	20020506	AU 2001-94628	20010919
JP 2004512336	T2	20040422	JP 2002-537736	20010919
US 2003028022	A1	20030206	US 2002-31812	20020328
US 6734191	B2	20040511		
NO 2003001161	A	20030313	NO 2003-1161	20030313
US 2004171638	A1	20040902	US 2004-799386	20040311
US 2004220207	A1	20041104	US 2004-858910	20040601
US 2005026942	A1	20050203	US 2004-914663	20040809
PRAI US 2000-234510P	P	20000922		
US 2000-234816P	P	20000922		
US 2000-232891P	P	20000915		
US 2000-233087P	P	20000915		
US 2001-957654	A3	20010917		
US 2001-957682	A3	20010917		
WO 2001-US29590	W	20010919		
US 2002-31812	A1	20020328		

OS MARPAT 136:355235
IT **422282-07-3P**, AMD 9986
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(chemokine receptor modulator; preparation of N-(tetrahydroquinolinyl)-N-(benzimidazolylmethyl)amines and analogs as chemokine receptor modulators for treatment of HIV or FIV)
RN 422282-07-3 CAPLUS
CN 1H-Imidazole-2,5-dimethanamine, N5-(1H-benzimidazol-2-ylmethyl)-1-(phenylmethyl)-N5-(5,6,7,8-tetrahydro-8-quinolinyl)-, tetrahydrobromide (9CI) (CA INDEX NAME)

1/30/06



●4 HBr

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT